

Package: slurmwiz (via r-universe)

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Type Package

Title Convert Raw Mass Spectrometry Files

Version 0.1.4

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Description Wrapper for converting raw mass spectrometry data files using the pwiz docker container through apptainer on a high performance computer (HPC) cluster running SLURM workload manager.

License GPL (>= 3)

Imports yaml, glue

Suggests pkgload, testthat (>= 3.0.0), withr

Config/testthat/edition 3

Encoding UTF-8

RoxygenNote 7.3.2

Roxygen list(markdown = TRUE)

Repository <https://aberhml.r-universe.dev>

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detect_file_type	<i>Detect File Type</i>
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Description

Detect the main file type in a directory of raw files

Usage

```
detect_file_type(input)
```

Arguments

input	the absolute file path of the directory of raw files for conversion
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Value

a character string of the file type for conversion

slurm_convert	<i>Convert Raw Files using msconvert and SLURM</i>
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Description

Convert raw mass spectrometry files using a combination of singularity, t

Usage

```
slurm_convert(input, output, format_out, conversion_args)
```

Arguments

input	the absolute file path of the directory of raw files for conversion
output	the absolute file path where converted data files will be saved to
format_out	a character string of msconvert format for conversion.
conversion_args	a character string of msconvert arguments without the --filter prefix (ie, peakPicking true 1-)

Examples

```
## Not run:
slurm_convert(input = 'hpc/storage/my_raw_data', output = 'hpc/home/my_converted_data', format_out = 'mzML', conv
## End(Not run)
```

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